

# Partial densities of electronic states in Al- or Mg-based complex intermetallics

Jean-Marie Dubois

Université de Lorraine and Jožef Stefan Institute, [jean-marie.dubois@univ-lorraine.fr](mailto:jean-marie.dubois@univ-lorraine.fr)

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# Partial densities of electronic states in Al- or Mg-based complex intermetallics

Jean-Marie Dubois

*Institut Jean Lamour (UMR 7198 CNRS-Université de Lorraine), 2 Allée André Guinier, BP 50840, F-54011 Nancy.*

*Jožef Stefan Institute, K7 Dpt for Nanostructured Materials, Jamova Cesta 39, SI-1000 Ljubljana.*

*Jean-marie.dubois@univ-lorraine.fr*

Soft X-ray emission spectroscopy (XES) is a unique technique that may be used to investigate separately Al s,d and Al p (Mg s,d and Mg p) states in solids of these elements with a very good energy resolution owing to the finite life time of the core hole created by electron excitation. It was extensively employed by Esther Belin-Ferré (EBF hereafter) with the aim to map both the valence and conduction sides of the electronic structure of selected complex compounds. The most salient results appeared out of a systematic study of quasicrystals (Al-Cu-Fe and Al-Pd-Mn) in comparison to crystals of related chemical composition, either binary compounds like  $\theta$ -Al<sub>2</sub>Cu or so-called approximants containing up to thousands atoms per unit cell.

In the interest of time, the talk will be restricted to a selection of the most important results of EBF, namely: i-evidence of the formation of a pseudo-gap at the Fermi energy in Al-based compounds and its correlation to the complexity of the atomic structure of the crystal (Fig. 1), ii-phase stability and transport properties of the same compounds in the light of the data gained about the Al-3p partial DOS, iii-formation and role on phase selection of d-states appearing close to, and below, the Fermi energy in Al- or Mg-containing compounds.

Accounting further for the lifetime achievements of EBF will not be possible in the context of this conference, but few key references<sup>3,4</sup> to her works will be provided.

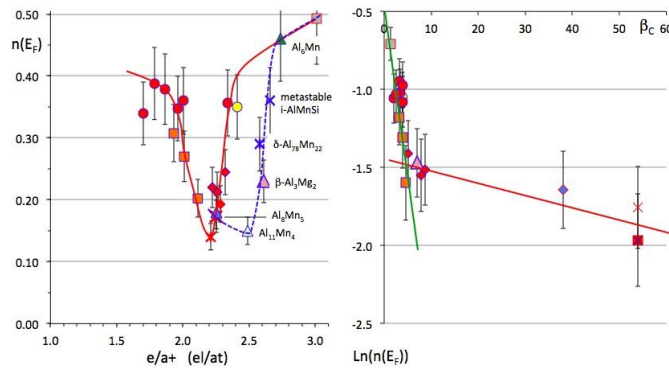


Fig. 1: Left: partial density of Al3p states measured by XES at the Fermi energy of a series of Al-Cu-Fe stable crystals and quasicrystals (data linked by a red line, to guide the eye) and binary Al-Mn and Al-Mg compounds (blue dashed line). The x-axis plots the e/a values corresponding to those compound compositions according to the e/a values for the individual constituents obtained by Mizutani and his co-workers<sup>1</sup>. Right: the same data in a log-log plot as a function of  $\beta_C = \ln(N_{UC})$  where  $N_{UC}$  is the number of atoms per unit cell. The index  $\beta_C$  yields for a definition of the complexity of the lattice<sup>2</sup>.

1. Role of electron concentration parameter  $e/a$  in energy-gap formation mechanism through interference phenomenon.

U. Mizutani and H. Sato, this conference.

2. Properties- and applications of quasicrystals and complex metallic alloys.

J.M. Dubois, Chem. Soc. Rev., 2012, 41, 6760–6777.

3. Electronic structure in quasicrystalline compounds and related crystals

E. Belin-Ferré, J. of Phys. Condensed Matter **14** R789-R817 (2002).

2. Study of Al-Cu Hume-Rothery alloys and their relationship to the electronic properties of quasicrystals.

V. Fournée, E. Belin-Ferré, J. M. Dubois, J. Phys.: Cond. Matter **10** 4231-4244 (1998).

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